Appendix A Life Estimation through Weibull Distribution

A.1 Introduction

Weibull proposed a distribution to describe the life length of materials under fatigue and fracture loads. Weibull developed this distribution to study fatigue and fracture of materials. The Weibull distribution is defined by a few parameters and estimation of these parameters for a given data set is necessary to describe the data set by the Weibull distribution.

Weibull distribution theory is a probable distribution which gives details of the lifetime characteristics of a particular part or service component. It is particularly emphasized on failure-rate. Weibull distribution is used throughout reliability engineering to anticipate and account for issues related to wear-out during development [184].

A.2 Weibull distribution for estimation of life prediction

Weibull proposed a distribution to describe the life length of materials under fatigue and fracture loads. According to this distribution, failure distribution can be described as [185]:

$$P_f = 1 - \exp\left[-\left(\frac{x - x_u}{x_0}\right)^m\right] \quad \text{for } x \geq x_u, x_0 > 0, m > 0 \qquad \text{(A.1)}$$

where x_0 is the scale parameter. It is the characteristic value of the distribution, such as time-to-failure or load. m is the shape parameter of the distribution or the Weibull modulus. It controls the width of the frequency distribution of the measured values of the parameters. The higher the value of the m, the narrower the distribution of the measured value and the higher its peak. x_u is called the location parameter which is the characteristic smallest value of the measured parameter. There is zero probability of failure if the applied stress or time-to-failure x is smaller than x_u .

The Weibull theory uses the weakest link approach to describe the strength of various materials where the strength of the weakest link determines the strength of the chain. Consequently, the measured value of the parameter is the minimum value (smallest value) from a set of possible values.

Equation (A.1) is a three parameter Weibull distribution. When location parameter is assumed to be zero, the resulting distribution is the two parameter Weibull distribution:

$$P_f = 1 - \exp\left[-\left(\frac{x}{x_0}\right)^m\right] \qquad \text{(A.2)}$$

This two parameter Weibull distribution has been used extensively where the minimum value of random variable may be assumed to be equal to zero. The probability density function of Weibull distribution is

$$f(x) = \frac{dP_f}{dx} = \frac{m}{x_0}\left(\frac{x}{x_0}\right)^{m-1} \exp\left[-\left(\frac{x}{x_0}\right)^m\right] \qquad \text{(A.3)}$$

Depending upon the values of m and x_0, the probability density function can take a wide variety of shapes. Rough estimation of the Weibull distribution parameters can also be made graphically by plotting Equation (A.2) after taking double algorithms and a suitable transformation. More accurate values of Weibull distribution parameters for a failure data set of specimens are estimated by following method:

1) Least square estimation (LSE)
2) Maximum likelihood method (MLM)

A.2.1 Least Square Estimation (LSE)

Equation (A.2) can be transformed into a linear form by rearranging the equation and taking logarithms of both sides twice:

$$\ln\ln\frac{1}{1-P_f} = m\ln x - m\ln x_0 \qquad \text{(A.4)}$$

The probability density function, P_f , for a given x can be calculated from n measured data after ordering such that $x_1 \le x_2 \le ... \le x_n$. Using order statistics of Wilks, an unbiased estimator of P_f is

$$P_f = \frac{i}{n+1} \qquad \text{(A.5)}$$

where i is the rank of the specimen in order of increasing measured value of x . Although there are other slightly different forms of P_f , the above form gives the minimum variance.

Substituting Equation (A.5) in Equation (A.2), we get

$$\ln\ln\frac{n+1}{n+1-i} = m\ln x - m\ln x_0 \qquad \text{(A.6)}$$

Both m and x_0 can be estimated by plotting $\ln\ln(n+1)/(n+1-i)$ against $\ln x$ and fitting the straight line. The Weibull parameter m is the slope of the best fit straight line. Although a line may be fitted graphically using eye-estimation, fitting the straight line using least-squares regression is generally preferred for accuracy of estimation. Equation (A.6) may be written as

$$y_i = \ln\ln\frac{n+1}{n+1-i} = m\ln x_i - m\ln x_0 + c_i \qquad \text{(A.7)}$$

where c_i is the error due to the difference between the observed value of $P_f(x_i)$ and its expected value.

A.2.2 Maximum Likelihood Method (MLM)

The Maximum likelihood method provides a procedure for deriving the estimates of the Weibull distribution parameters directly. A random variable x following the Weibull distribution has a probability density function $f(x;m,x_0)$ with Weibull parameters m and x_0 as given in Equation (A.3). The likelihood of obtaining particular sample value x_i may be assumed to be proportional to the probability density function at x_i. Hence, the likelihood of obtaining n independent observations $x_1, x_2, ..., x_n$ is

$$L(x_1,...,x_n;m,x_0) = f(x_1;m,x_0)\,f(x_2;m,x_0)...f(x_n;m,x_0) = \prod_{i=1}^{n} f(x_i;m,x_0) \qquad \text{(A.8)}$$

L is the likelihood function of the data set $x_1, x_2, ..., x_n$. The maximum-likelihood estimator of m and x_0 will then be the particular values of m and x_0 so that L or the probability of obtaining the data set is maximized. Due to the multiplicative nature of L, it is generally more convenient to maximize the logarithm of the likelihood function instead

$$\frac{\partial \ln L(x_1,...,x_n;m,x_0)}{\partial m} = 0 \qquad \text{(A.9)}$$

and

$$\frac{\partial \ln L(x_1,...,x_n;m,x_0)}{\partial x_0} = 0 \qquad \text{(A.10)}$$

The maximum-likelihood function of Weibull distribution can be written by substituting Equation (A.3) in Equation (A.8);

$$L = \frac{m^n}{x_0^n}\left(\frac{x_1}{x_0}\right)^{m-1}\left(\frac{x_1}{x_0}\right)^{m-1}\cdots\left(\frac{x_1}{x_0}\right)^{m-1} * \exp\left[-\left(\frac{x_1}{x_0}\right)^{m}\right]\exp\left[-\left(\frac{x_2}{x_0}\right)^{m}\right]\cdots\exp\left[-\left(\frac{x_n}{x_0}\right)^{m}\right] \quad \text{(A.11)}$$

Taking the logarithm on both sides and rearranging the terms,

$$\ln(L) = n\ln m - n\ln x_0 + (m-1)\sum_{i=1}^{m}\ln\left(\frac{x_i}{x_0}\right) - \sum_{i=1}^{n}\ln\left(\frac{x_i}{x_0}\right)^{m} \quad \text{(A.12)}$$

Taking the derivative of $\ln(L)$ with respect to x_0 and equating it to zero, we get

$$x_0^m = \frac{1}{n}\sum_{i=1}^{n} x_i^m \quad \text{(A.13)}$$

Similarly, equating the derivative of $\ln(L)$ with respect to m to zero, we get

$$\frac{n}{m} - n\ln x_0 + \sum_{i=1}^{n}\ln x_i - \sum_{i=1}^{n}\left(\frac{x_i}{x_0}\right)^{m}\ln\left(\frac{x_i}{x_0}\right) = 0 \quad \text{(A.14)}$$

Substituting Equation (A.13) in Equation (A.14), we get

$$\frac{n}{m} + \sum_{i=1}^{n}\ln x_i - n\frac{\sum_{i=1}^{n}(x_i^m \ln x_i)}{\sum_{i=1}^{n} x_i^m} = 0 \quad \text{(A.15)}$$

Equation (A.15) can be solved for m using the Newton-Raphson iterative method. This method requires evaluation of both the function and its derivative at different points. One of the significant advantages of this method is that it converges quadratically. The number of significant digits approximately doubles at each step near a root of the equation.

According to Newton-Raphson method,

$$m_{k+1} = m_k - \frac{f(m_k)}{f'(m_k)} \quad \text{(A.16)}$$

where $f(m_k)$ is the left side of Equation (A.15) at the kth iteration of m. Since $f'(m_k)$ is $df(m_k)/dm_k$, $f'(m_k)$ is given by

$$f'(m_k) = -\frac{n}{m_k^2} - \frac{n\sum_{i=1}^{n} x_i^{m_k} \sum_{i=1}^{n} [x_i^{m_k} (\ln x_i)^2] - n[\sum_{i=1}^{n} (x_i^{m_k} \ln x_i)]^2}{[\sum_{i=1}^{n} x_i^{m_k}]^2} \tag{A.17}$$

Therefore, m_{k+1} can be calculated from

$$m_{k+1} = m_k - \frac{\{1/m_k\} + \{1/n\}\{\sum_{i=1}^{n} \ln x_i\} - \{\sum_{i=1}^{n} [x_i^{m_k} \ln x_i]/\sum_{i=1}^{n} x_i^{m_k}\}}{-\{1/m_k^2\} - \{\sum_{i=1}^{n} x_i^{m_k} \sum_{i=1}^{n} [x_i^{n} (\ln x_i)^2] - [\sum_{i=1}^{n} (x_i^{m_k} \ln x_i)]^2\}/[\sum_{i=1}^{n} x_i^{m_k}]^2} \tag{A.18}$$

From an initial guess of m, the value of Weibull modulus m can be estimated when the difference between subsequent iterations is less than a predefined tolerance value.

A.3 Parameters of Weibull distribution function

The case where $x = 0$ and $x_0 = 1$ is called the standard Weibull distribution. The case where $x = 0$ is called the 2-parameter Weibull distribution. The equation for the standard Weibull distribution reduces to

$$f(x) = mx^{(m-1)} \exp(-(x^m)), x \ge 0; m > 0 \tag{A.19}$$

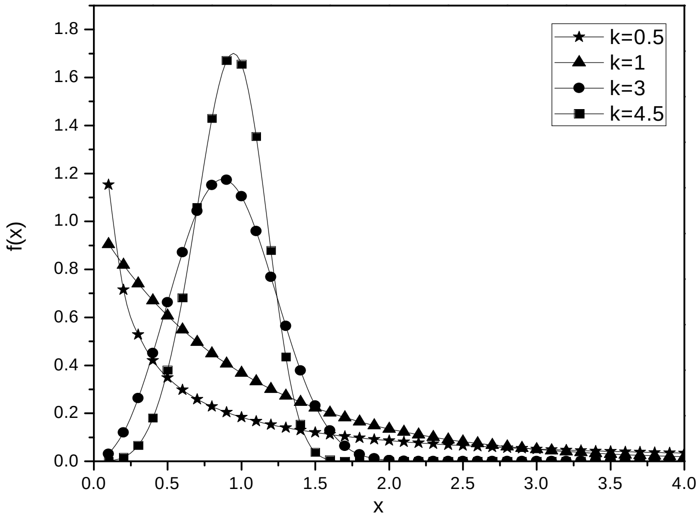

Figure A.1 Weibull Probability Density Function

The curve of the function varies greatly depending on the numerical values of parameters. Most important is the shape parameter, '*m*', which reflects the pattern of curve. Note that when '*m*' is 1.0, the Weibull function reduces to the Exponential and that when '*m*' is about 3.5 (and x_0 1, x 0), the Weibull closely approximates the Normal distribution. In practice, '*m*' varies from about 1/3 to 5. The scale parameter 'x_0' is related to the peakedness of the curve, i.e., as 'x_0' changes, the curve becomes flatter of more peaked. The location parameter 'x ' is the smallest possible value of 'x'. This is often assumed to be 0, thereby simplifying the equation. Figure A.1 shows the variation of function for different values of shape parameter, considering x 0 and x_0 1.

The Weibull covers many shapes of distributions. This makes it popular in practice because it reduces the problems of examining a set of the common distributions (example: normal or exponential) fits best.

The Weibull distribution gives a distribution for which the failure rate is proportional to power of time (Figure A.2).

If m 1, failure rate decreases over time

If m 1, failure rate is constant over time

If m 1, failure rate increases over time

In the field of material science, 'm' is a distribution of strength known as Weibull Modulus.

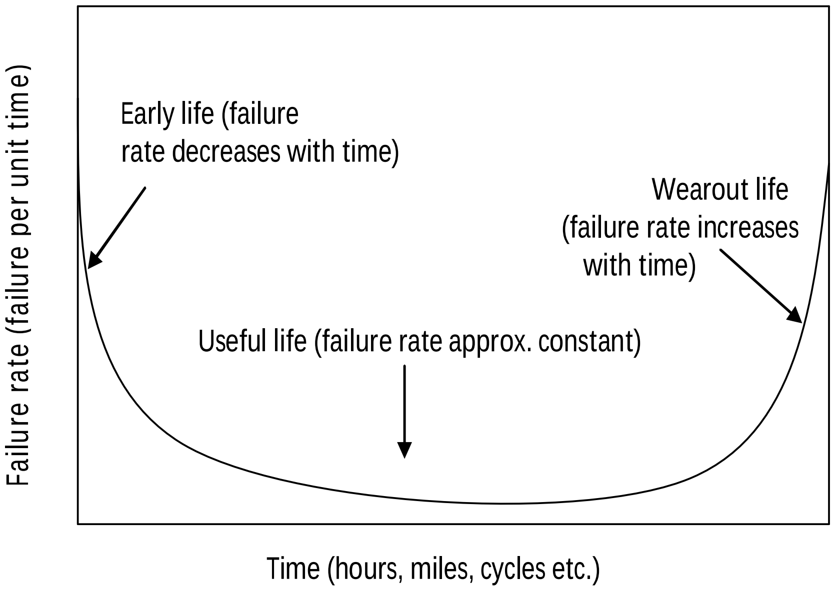

Figure A.2 Weibull Failure Rate for 0<m<1, m=1, m>1

Graphite is similar to the ceramic materials in some respects that it is not processed via melting [186,187]. Some of the important characteristics of graphite are its strength at high temperature, high thermal conductivity and shock resistance, fire proof and acid and alkaline proof. It is similar to other brittle materials in some respect that it does not exhibit plastic deformation and show wide scatter in strength. It has a non-linear stress-strain response and this behavior is different in tension than in compression. This is because of the distributed damage and damage accumulation within the material prior to rupture. This type of material is known as known as quasi-brittle material [188,189].

The fracture of graphite can be a complex process, with different grades of graphite potentially having different failure behaviors. Fracture is nominally brittle or quasi-brittle, with little or no plasticity prior to failure. This means that fracture is influenced by pre-existing flaws or inherently weak regions in the material. Porosity can also be an important factor for fracture. Tensile fracture occurs when a local concentration of micro-cracks develop and coalesce to form an unstable micro-crack of critical size. Tucker and McLchlan [190] discussed the micro-growth tends to be trans-granular (through the grains), with the crack path within the individual grain corresponding to the crystalline cleavage plane [191,192].

So the failure and life estimation of the graphite can be easily done by Weibull distribution (Equation A.1). This chapter presents the estimation of Weibull parameters by Least Square Method and Maximum Likelihood Method. A computer program has been developed for the analysis of two parameter Weibull distribution. It is illustrated that maximum likelihood estimator gives more accurate values of Weibull model in comparison to least square estimation. Rough estimation method of Weibull parameters is extended to the more accurate methods for nuclear grade-graphite specimen data [193] for fatigue and fracture characterization of graphite claded nuclear reactor.

A.4 Problem formulation

The estimation of shape and scale parameters of Weibull distribution is carried out by using least square and maximum likelihood methods. Experimental data of graphite is used for evaluation and then the value of shape parameter evaluated by different methods is compared with the result given in Price paper [193].

Price conducted more than 2000 ambient temperature tensile tests on H-451 nuclear grade graphite specimen. Four 127mm deep slabs were cut transverse to the axis. Two slabs (1 and 4) were located within 25mm of the two ends of the log, and two slabs (2 and 3) were located adjacent to the mid-length plane of the log. Each slab was cut into an edge section and center section on a radius of 108mm along the centerline axis of the log. Test specimens were core drilled in the axial (with grain) and radial (against grain) orientations from the central zone and the edge zone of each slab.

A.5 Results and discussion

Figures A.3 and A.4 represent the plots of failure stress data of axial and radial orientations, respectively. These plots are for the determination of Weibull parameters using Least Square Estimation method. Figures show the best fit line graph for a particular location each in axial and radial orientations. This type of graph is drawn for all location in both orientations to evaluate the shape and scale parameters. The adjusted R-square value for all graphs is more than 95%, which shows that the parameters are accurately determined. Also, in case of Maximum Likelihood Method, a program is developed in FORTRAN to estimate the Weibull parameters. Tables A.1 and A.2 show the results of shape and scale parameters of small tensile specimen at different locations using different methods for axial and radial orientations, respectively.

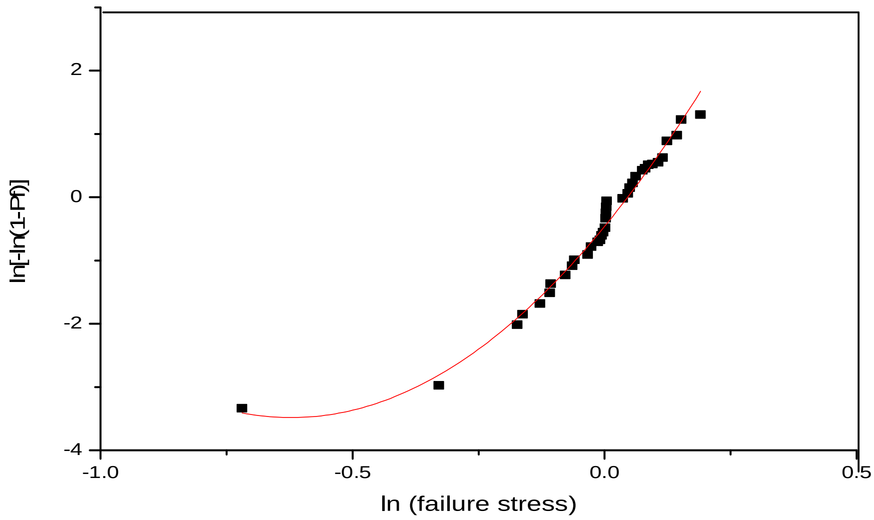

Figure A.3 Plot of failure stress data for axial orientaion

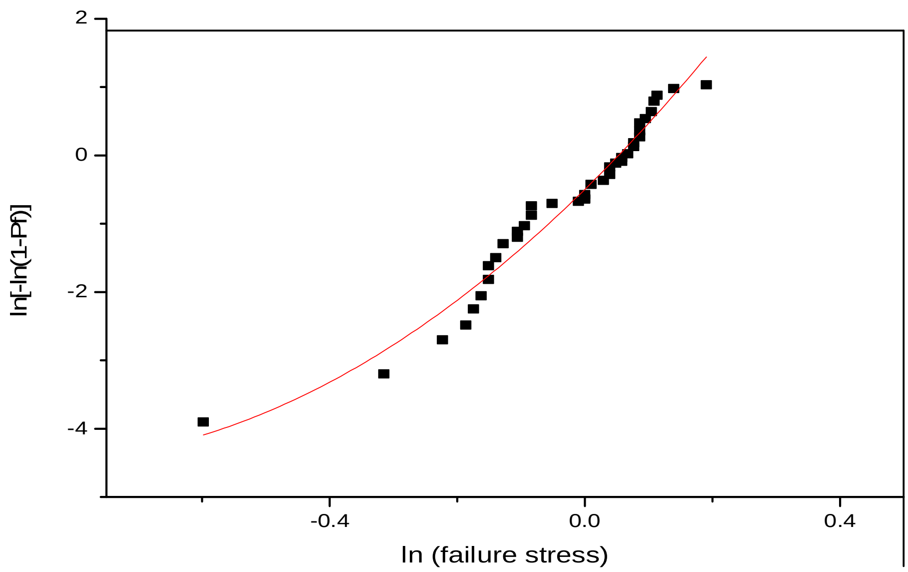

Figure A.4 Plot of failure stress data for radial orientation

Table A.1 Comparison of estimated values of Weibull parameters (axial orientation)

Locations	Methods of estimation	Shape parameter	Scale parameter
End edge 1	Analytically (Price, 1976)	9.4	-

	LSE	9.2	1.058
	MLM	10.3	1.057
End edge 4	Analytically (Price, 1976)	10.0	-
	LSE	9.35	1.1
	MLM	9.19	1.08
End centre 1	Analytically (Price, 1976)	7.5	-
	LSE	6.8	1.07
	MLM	7.99	1.02
End centre 4	Analytically (Price, 1976)	8.2	-
	LSE	7.56	1.1
	MLM	8.08	1.07
Mid length edge 2	Analytically (Price, 1976)	12.6	-
	LSE	12.09	1.07
	MLM	12.05	1.06
Mid length edge 3	Analytically (Price, 1976)	10.0	-
	LSE	9.18	1.05
	MLM	9.71	1.05
Mid length centre 2	Analytically (Price, 1976)	13.4	-
	LSE	13.16	1.04
	MLM	13.26	1.04
Mid length centre 3	Analytically (Price, 1976)	6.8	-
	LSE	6.31	1.05
	MLM	7.2	1.04

Table A.2 Comparison of estimated values of Weibull parameters (radial orientation)

Locations	Methods of estimation	Shape parameter	Scale parameter
End edge 1	Analytically (Price, 1976)	7.2	-
	LSE	7.02	1.03
	MLM	8.27	1.02
End edge 4	Analytically (Price, 1976)	9.9	-
	LSE	9.45	1.04
	MLM	10.2	1.05
End centre 1	Analytically (Price, 1976)	6.2	-

	LSE	6.7	1.11
	MLM	6.13	1.109
End centre 4	Analytically (Price, 1976)	7.2	-
	LSE	7.6	1.05
	MLM	7.9	1.03
Mid length edge 2	Analytically (Price, 1976)	9.7	-
	LSE	9.3	1.04
	MLM	10.02	1.04
Mid length edge 3	Analytically (Price, 1976)	6.8	-
	LSE	5.77	1.01
	MLM	6.9	0.99
Mid length centre 2	Analytically (Price, 1976)	4.6	-
	LSE	4.45	1.06
	MLM	5.7	1.04
Mid length centre 3	Analytically (Price, 1976)	8.3	-
	LSE	8.12	1.05
	MLM	9.7	1.05

Tables show the evaluated parameters of two parameter Weibull distribution using Least Square method and Maximum Likelihood method. The parameters are calculated for all the four slabs including the edge and centre. These values are then compared with the results given in Price paper which is calculated analytically. By using the least square and maximum likelihood methods, both shape and scale parameters are estimated. While in Price paper, the values of slope parameter are only given. It is found that in both axial and radial orientation, the various values of Weibull modulus are nearly same with the referred paper results for all locations. By comparing these values, it can be said that modulus value is somewhat larger in case of MLM compared to LSE. The reason of larger value is that it determines the value accurately.

It is seen that the modulus is more for the slabs 2 and 3 compared to slabs 1 and 4 for axial orientation. This means that modulus value is more for mid length than end. Moreover, these values are larger in case of slab 2 than of slab 3. The maximum value is for the locations mid length edge 2 and mid length centre 2 and minimum for locations end centre 1 and mid length centre 3.

In case of radial orientation, minimum value of Weibull modulus is for mid length centre 2. This is the smallest value in both axial and radial orientations. The maximum value is in case of end edge 4.

Then the values of scale parameter calculated from LSE and MLM are compared. In both axial and radial orientation case, these values are almost same and they are nearly equal to one.

A.6 Conclusion

A computer program has been developed to estimate the values of the modulus and scale parameter of Weibull model for tensile specimen nuclear graphite data using least square and maximum likelihood methods. These parameters have been compared with results given in referred paper and it is found that they are matched well. Following points can be concluded through the result:

1. It has been found that parameters are accurately determined by maximum likelihood method among all methods.
2. The value of shape parameter determined by maximum likelihood method is larger compared to analytical and least square estimation.
3. Scale parameter evaluated thorough maximum likelihood and least square methods are approximately same and its value is nearly equal to one.

This procedure can be extended for future work.

Appendix B List of Publications

1. Saumya Shah and S.K. Panda: "Bimodularity of interface layer and curing stress coupling effects on mixed mode fracture behaviour of functionally graded tee joint", International Journal of Adhesion and Adhesives, vol. 75, pp. 74-87, 2017. (*Publisher: Elsevier; Impact Factor: 2.211*)

2. Saumya Shah and S.K. Panda: "Thermoelastic fracture behaviour of bimodular functionally graded skin-stiffener composite panel with embedded interlaminar delamination", Journal of Reinforced Plastics and Composites, DOI: 10.1177/0731684417709951. (*Publisher: SAGE; Impact Factor: 1.086*)

3. Saumya Shah, S.K. Panda and D.Khan: "Analytical Solution for a Flexural Bimodulus Beam", Emerging Materials Research, vol. 6, pp. 1-30, 2017. (*Publisher: ICE Virtual Library; Impact Factor: 0.313*)

4. Saumya Shah, S.K. Panda and D. Khan: "Weibull Analysis of H-451 Nuclear-Grade Graphite", Procedia Engineering, vol. 144, pp. 366-373, 2016. (*Publisher: Elsevier; Scopus*)